1-Pentanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,5-undecafluoro-

2706-91-4 | DTXSID8062600

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 5.73

Global applicability domain: Outside

Local applicability domain index: 2.32e-01

Confidence level: 7.97e-01

Nearest Neighbors from the Training Set

Image not found
4-Hydroxy-1-naphthalenesulfonic
acid monosodium salt
Measured: 12.9
Predicted: 6.33

Image not found
2-Amino-1-naphthalenesulfonic
acid
Measured: 6.03
Predicted: 6.40

Image not found
4-Amino-1-naphthalenesulfonic
acid sodium salt
Measured: 6.03
Predicted: 5.38

Image not found
2-Amino-5-
methylbenzenesulfonic acid
Measured: 3.98
Predicted: 6.29

Image not found
Benzenesulfonic acid, 2-chloro-
5-nitro-, sodium salt
Measured: 3.02
Predicted: 5.14